

1,4,7-trimethyl-dibenzothiophene

Other names: Dibenzothiophene, 1,4,7-trimethyl
Inchi: InChI=1S/C15H14S/c1-9-4-7-12-13(8-9)16-15-11(3)6-5-10(2)14(12)15/h4-8H,1-3H3
InchiKey: CXSJRPQUOLEFR-UHFFFAOYSA-N
Formula: C15H14S
SMILES: Cc1ccc2c(c1)sc1c(C)ccc(C)c12
Mol. weight [g/mol]: 226.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.27		Crippen Method
logp	4.980		Crippen Method
mcvol	180.180	ml/mol	McGowan Method
rinpol	2189.00		NIST Webbook
rinpol	352.62		NIST Webbook
rinpol	350.56		NIST Webbook
rinpol	352.62		NIST Webbook
rinpol	2189.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R192982&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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